National Certificate of Educational Achievement
TAUMATA MĀTAURANGA Ā-MOTU KUA TAEA

Exemplar for Internal Achievement Standard

Chemistry Level 3

This exemplar supports assessment against:

Achievement Standard 91388

Demonstrate understanding of spectroscopic data in chemistry.

An annotated exemplar is an extract of student evidence, with a commentary, to explain key aspects of the standard. It assists teachers to make assessment judgements at the grade boundaries.

New Zealand Qualifications Authority

To support internal assessment

	Grade Boundary: Low Excellence
1.	For Excellence, the student needs to demonstrate comprehensive understanding of spectroscopic data in chemistry. This involves justifying the structure of organic molecules by integrating spectroscopic data. This student has integrated the three types of spectroscopic data to justify the identification of the unknown molecule (1). For a more secure Excellence, the student could explain how other molecules were excluded based upon the information from the spectroscopic data supplied.

Student 1: Low Excellence

NZQA Intended for teacher use only

Mass Spec:

m/z ratio	group
88	C_2H_4O is the empirical formula and has a mass of 44 so compound must have formula $C_4H_8O_2$. This is the molecular ion peak. And the base peak as it has 100% absorbance.
89	Peak due to relative isotopic abundance of ^{13}C isotope
45	$COOH^+$
43	$C_3H_5^+$
29	C_2H_5

IR:

Wavenumber(cm^{-1})	Characteristic group
2980 broad	Carboxylic acid
1710 sharp	C=O Aldehydes, ketones, carboxylic acids, esters

NMR:

Chemical shift (ppm)	Characteristic group
13	CH_3
19	CH_2
38	CH_2
180	C downfield shift due to C bonded to highly electronegative atom or atoms

There are 4 carbons in the compound

Justification:

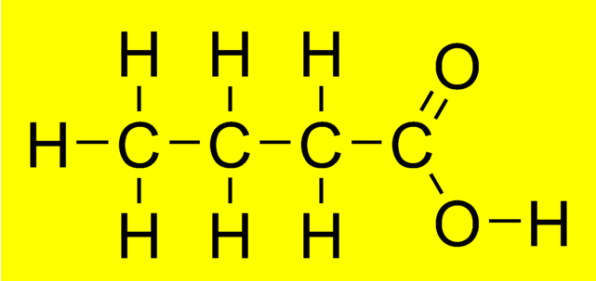
With the mass spectrum showing a peak at 88 and an empirical formula of C_2H_4O the chemical formula of the compound is $C_4H_8O_2$. The peak at 29 is characteristic of a fragment formed due to the breakup of the compound in the mass spectrometer to form a $C_2H_5^+$ion. The peak at 89 is due to isotopic abundance of the ^{13}C and will give peaks with an increased mass of 1 due to its presence in the compound. The peak at 45 is due to the $COOH^+$ ion following fragmentation as is the peak at 43 due to the $C_3H_5^+$ ion. This indicates that compound A could be butanoic acid.

1

The 4 different chemical shifts indicating that the carbons are all in different environments in the ^{13}C spectra suggest that the compound would be the straight chain butanoic acid. The peak at 180 would be due to the carbon with two oxygen atoms bonded to it. The peak at 13 is likely to be the C of the CH_3 group as this would be expected furthest up field and peaks at 19 and 38 due to the CH_2 groups between the CH_3 and the COOH group in the straight chain compound,

Analysis of the IR spectra shows a broad peak at 2980 cm^{-1} confirming the presence of the O-H group on the butanoic acid. The acid is further confirmed by the peak at 1750cm^{-1} which is characteristic of the C=O.

The structure of A is shown below. A is butanoic acid.



	Grade Boundary: High Merit
2.	For Merit, the student needs to demonstrate in-depth understanding of spectroscopic data in chemistry. This involves determining the structure of organic molecules using spectroscopic data. This student has explained how the three types of spectroscopic data were used to identify the molecule (1). To reach Excellence, the student could intergrate more of the identified data to justify the identification of the molecule.

Student 2: High Merit

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Mass Spec:

m/z ratio	group
88	C_2H_4O is the empirical formula and has a mass of 44 so compound must have formula $C_4H_8O_2$. This is the molecular ion peak. And the base peak as it has 100% absorbance.
89	Peak due to relative isotopic abundance of ^{13}C isotope
45	$COOH^+$
43	$C_3H_5^+$
29	C_2H_5

IR:

Wavenumber(cm^{-1})	Characteristic group
2980 broad	Carboxylic acid
1710 sharp	C=O Aldehydes, ketones, carboxylic acids, esters

NMR:

Chemical shift (ppm)	Characteristic group
13	CH_3
19	CH_2
38	CH_2
180	C downfield shift due to C bonded to highly electronegative atom or atoms

There are 4 carbons in the compound

Justification:

With the mass spectrum showing a peak at 88 and an empirical formula of C_2H_4O the chemical formula of the compound is $C_4H_8O_2$. The peak at 29 is characteristic of a fragment formed due to the breakup of the compound in the mass spectrometer to form a $C_2H_5^+$ion. The peak at 45 is due to the $COOH^+$ ion. This indicates that compound A could be butanoic acid.

1

The 4 different chemical shifts indicating that the carbons are all in different environments in the ^{13}C spectra suggest that the compound would be the straight chain butanoic acid. The peak at 180 would be due to the carbon with two oxygen atoms bonded to it.

Analysis of the IR spectra shows a broad peak at 2980 cm^{-1} confirming the presence of the O-H group on the butanoic acid. The acid is further confirmed by the peak at 1750cm^{-1} which is characteristic of the C=O.

This makes me believe the molecule is butanoic acid.

	Grade Boundary: Low Merit
3.	For Merit, the student needs to demonstrate in-depth understanding of spectroscopic data in chemistry. This involves determining the structure of organic molecules using spectroscopic data. This student has identified a possible structure using some of the identified data from two types of spectroscopic data (1). For a more secure Merit, the student could explain how the identified data supports the identification of the molecule.

Student 3: Low Merit

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Mass Spec:

m/z ratio	group
88	C_2H_4O is the empirical formula and has a mass of 44 so compound must have formula $C_4H_8O_2$. This is the molecular ion peak.
45	COOH
29	C_2H_5

IR:

Wavenumber(cm^{-1})	Characteristic group
2980 broad	
1710 sharp	C=O

NMR:

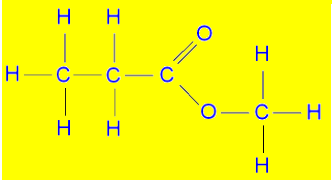
Chemical shift (ppm)	Characteristic group
13	C
19	C
38	C
180	C downfield shift due to bonding to electronegative atom oxygen.

There are 4 carbons in the compound

Justification

With the mass spectrum showing a peak at 88 and an empirical formula of C_2H_4O the chemical formula of the compound is $C_4H_8O_2$. The peak at 29 is characteristic of a fragment formed due to the breakup of the compound in the mass spectrometer to form a $C_2H_5^+$ion. The 4 different chemical shifts indicating that the carbons are all in different environments. The peak at 180 would be due to the carbon with two oxygens bonded to it. This is consistent with the ester methyl propanoate which would have 4 different carbon environments.

1



	Grade Boundary: High Achieved
4.	For Achieved, the student needs to demonstrate understanding of spectroscopic data in chemistry. This involves identifying discrete aspects of the structure of organic molecules using teacher-provided spectroscopic data. This student has identified discrete aspects of the spectroscopic data (1) and has used some of the spectroscopic data to identify a possible structure (2). To reach Merit, the student could explain how two different types of spectroscopic data result in the identification of the molecules structure.

Student 4: High Achieved

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Mass Spec:

m/z ratio	group
88	C_2H_4O is the empirical formula and has a mass of 44 so compound must have formula $C_4H_8O_2$. This is the molecular ion peak

IR:

Wavenumber(cm^{-1})	Characteristic group
2980 broad	
1710 sharp	C=O

1

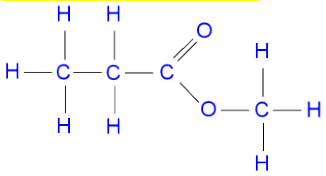
NMR:

Chemical shift (ppm)	Characteristic group
13	C
19	C
38	C
180	C

There are 4 carbons in the compound

From the three graphs the unknown compound is methyl propanoate which would have 4 different carbon environments.

2



	Grade Boundary: Low Achieved
5.	For Achieved, the student needs to demonstrate understanding of spectroscopic data in chemistry. This involves identifying discrete aspects of the structure of organic molecules using teacher-provided spectroscopic data. This student has identified discrete aspects from all three types of spectroscopic data (1). For a more secure Achieved, the student could identify what functional group that relates to the peaks on the infrared (IR) graph.

Student 5: Low Achieved

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Mass Spec

m/z ratio	group
88	C_2H_4O is the empirical formula and has a mass of 44 so compound must have formula $C_4H_8O_2$

1

IR:

Wavenumber(cm^{-1})	Characteristic group
2980 broad	-OH
1710 sharp	C=O

NMR:

There are 4 carbons in the molecule.

	Grade Boundary: High Not Achieved
6.	For Achieved, the student needs to demonstrate understanding of spectroscopic data in chemistry. This involves identifying discrete aspects of the structure of organic molecules using teacher-provided spectroscopic data. This student has identified some discrete aspects of two spectroscopic techniques (1). To reach Achieved, the student could identify the main peaks on the infrared (IR) graph, use the mass spectroscopy data to identify the molecular formula and use the NMR to identify the number of unique carbon environments.

Student 6: High Not Achieved

NZQA Intended for teacher use only

Mass Spec:

m/z ratio	group
88	This is the mass of the compound, 88gmol^{-1}

1

IR:

Wavenumber(cm^{-1})	Characteristic group
2980 broad	Acid

NMR: